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A FFT-based formulation for discrete dislocation dynamics in heterogeneous media

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ABSTRACT

In this paper, an extension of the DDD-FFT approach presented in [1] is developed for heterogeneous elasticity. For such a purpose, an iterative spectral formulation in which convolutions are calculated in the Fourier space is developed to solve for the mechanical state associated with the discrete eigenstrain-based microstructural representation. With this, the heterogeneous DDD-FFT approach is capable of treating anisotropic and heterogeneous elasticity in a computationally efficient manner. In addition, a GPU implementation is presented to allow for further acceleration. As a first example, the approach is used to investigate the interaction between dislocations and second-phase particles, thereby demonstrating its ability to inherently incorporate image forces arising from elastic inhomogeneities.

1. Introduction

In the recent years, Discrete Dislocation Dynamics (DDD) simulation, aiming at simulating the collective motion and interactions of large ensembles of dislocations, has proven to be a powerful tool to study plasticity at small scales [2–5]. Of particular interest, DDD simulations have permitted to extract critical parameters on the collective effects of dislocations behavior, thereby allowing to inform and delineate higher-scale models. Successful applications for instance include the quantification of latent-hardening effects in cubic [6–8] and hexagonal [9,10] crystals, the delineation of physical constitutive models for slip-driven plasticity [11–14], the quantification of the effect of dislocation interaction with irradiation-induced damage on strength [15–17], the investigation of plasticity in polycrystalline materials [18,19] and the computation of effective activation barrier pertaining to the bypass of randomly distributed obstacles [20,21].

From a general perspective, the dislocation network in DDD simulations is usually discretized into a series of interconnected segments. From there, the motion and interactions of dislocation segments is determined by calculation of the driving force acting on the dislocation lines. Since every dislocation segment elastically interacts with all other segments in the simulation volume through their stress field, forces are usually calculated following the superposition method by virtue of which individual elastic interaction forces on pairs of segments are added [22]. In the case of isotropic homogeneous media, analytical expressions, based on Mura's derivation [23], have been conveniently obtained [5,24] to quantify the interaction forces between segments. These analytical expressions have allowed to significantly reduce the computational cost associated with the calculation of segment–segment elastic interactions. However, in the case of heterogeneous media, ad-

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ditional image forces arise from the elastic and plastic mismatch between the different phases, for which no general closed form solution exists. As a result, costly expressions have been obtained for calculating the stress of dislocation segments in elastically heterogeneous media. Furthermore, these are limited to simple geometrical configurations such as bi-layered materials [25,26], thereby precluding the incorporation of second-phase inclusions with complex morphologies.

To alleviate the difficulties associated with the treatment of elastic interactions between dislocations and second-phase inclusions, several phenomenological approaches have first been incorporated in DDD simulations. Naturally these approaches necessarily entail that approximations are made. For instance, simple line tension approximations were used to study particles strengthening as a function of particles spacing [27], size [28] and strength [29,30]. Incorporating more details, Mohles et al. successfully studied the propagation of dislocation lines within an array of coherent and incoherent shearable particles using DDD simulations in which obstacles were modeled by a supplementary stress contribution arising from an antiphase boundary energy density [31–33]. While this supplementary contribution was added to the Peach–Koehler force on dislocation lines inside the particles, it was not considered outside of the particles, such that elastic interaction effects were effectively ignored. Similarly, in the work of Queyreau and co-workers where the Orowan by-passing mechanism on incoherent carbides was studied in BCC steels, no stress field was associated to the impenetrable obstacles [34]. More recently, DDD was used in [17] to assess the validity of particle-hardening models for a combination of voids and self-interstitial atom loops. In this last work, elastic interactions with voids were modeled using an atomistically-informed breakaway angle. Originally, in work by Monnet et al. [35] the description of the interaction between a Cr precipitate and a glide dislocation was parameterized from atomistic simulations. A key advantage here lies in the capability of the approach to include temperature effects. However, as discussed in [21,35], as one is necessarily limited to studying a few geometrical defect configurations via atomistic simulations, the direct parameterization into DDD as done in [17,35] for example, can yield effective behaviors that are not statistically representative.

Focus is placed here on the treatment of the effects of elastic heterogeneity. In this regard, a few DDD simulations have readily incorporated inclusions elastic interaction effects. Two different approaches – both relying on the Finite Element Method (FEM) – have been proposed thus far. The first method was developed in the seminal work of Shin and co-workers [36–38]. In their approach, the superposition method proposed by Van der Giessen and Needleman [22] was further extended to account for second-phase elastic inclusions in the matrix. By coupling the DDD simulations to a FEM code, the heterogeneous stress field generated by the elastic mismatch between the matrix and the precipitate was accounted for in the form of image forces, and the interaction of dislocations with cubical [36] and spherical [37] precipitates was investigated. Using the same superposition approach, interaction forces between a straight dislocation line and spherical particles [39] and voids [40] were calculated. However, this method is computationally intensive as per the fine FEM meshes required. Most studies relying on the use of the superposition principle have therefore been limited to the investigation of static or relaxed configurations, and the approach might become intractable when performing dynamic simulations up to relevant levels of strain. As an alternative approach to the problem, the Discrete continuous model – hereafter DCM-FEM – introduced by Lemarchand and co-workers [41] and relying on an eigenstrain formalism was used to model the plastic deformation in metal matrix composites [42], and investigate plasticity in nickel-based single-crystal superalloys in which matrix channels were formed by the presence of precipitate phases [43,44]. However, although inherently accounting for heterogeneous elasticity, the DCM-FEM approach is practically limited to a coarse representation of precipitates (due to its computational cost) and cannot be employed to finely model particles.

In light of the above, current DDD approaches need to be refined and their limitations need to be addressed so as to (1) incorporate more details when studying interactions between second phases and dislocations, (2) extend their time and length scales such that refined models to be incorporated at the constitutive level can be delineated. Particularly, an accurate and efficient treatment of image forces arising from the elastic mismatch between the matrix and the particles needs to be incorporated. For this purpose, and to address the limitations of current approaches, an heterogeneous extension of the eigenstrain-based DDD-FFT approach recently introduced in [1] is proposed in this work. It is expected that a fine level of details can be incorporated in a computationally efficient manner, so as provide a numerical tool capable of accurately simulating the interactions between dislocations and second phases in heterogeneous anisotropic media. Furthermore, the current approach provides a general framework for heterogeneous elasticity, thereby paving the way towards performing DDD simulations in polycrystalline materials.

This paper is organized as follows. First, the implicit heterogeneous FFT-based formulation is presented in Section 2, and the different numerical schemes to solve for the mechanical state are detailed in Section 3. Then, details on the numerical implementation are given in Section 4 and a GPU-accelerated version of the FFT-based solver is proposed. In Section 5, the ability of the method to inherently account for the effects of elastic mismatches in heterogeneous media is demonstrated through static and dynamic configurations in which a dislocation is inserted into a two-phase material. Finally, the numerical efficiency of the approach is discussed in Section 6 and a conclusion is given in Section 7.

2. Heterogeneous FFT-based formulation for DDD

2.1. Dislocation motion

Considering an overdamped regime, the velocity $\vec{\boldsymbol{v}}$ of a dislocation line can be linearly related to the force on each dislocation segment $\vec{\boldsymbol{f}}$ through the mobility function $\mathcal{M}$: